Chemical Engineering and Technology 2018 vol.41 N8, pages 1604-1612

Thermodynamics of Imidazolium-Based Ionic Liquids Containing the Trifluoromethanesulfonate Anion

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2018 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim A thermochemical investigation of the series of 1-alkyl-3-methylimidazolium ionic liquids (ILs) with the trifluromethanesulfonate CF3SO3− anion is presented. Absolute vapor pressures and vaporization enthalpies were measured by using a quartz crystal microbalance (QCM). The enthalpies of solutions were determined by solution calorimetry. Gas-phase enthalpies of the formation of ILs were calculated by applying the high-level quantum-chemical method G3MP2. From a combination of experimental and theoretical results, the enthalpy of formation of aqueous CF3SO3− anion was derived for the first time.

http://dx.doi.org/10.1002/ceat.201700454

Keywords

Enthalpy of formation, Enthalpy of vaporization, Ionic liquids, Thermodynamics, Vapor pressure

References

[1] S. Liang, W. Chen, K. Cheng, Y. Guo, X. Gui, in Applications of Ionic Liquids in Science and Technology (Ed.: P. S. Hardy), InTechOpen, London 2011, 467–494

[2] F. Heym, J. Haber, W. Korth, B. J. M. Etzold, A. Jess, Chem. Eng. Technol. 2010, 33, 1625–1634

[3] N. V. Ignat'ev, P. Barthen, A. Kucheryna, H. Willner, P. Sartori, Molecules 2012, 17, 5319–5338. DOI: 10.3390/molecules17055319

[4] R. P. Swatloski, S. K. Spear, J. D. Holbrey, R. D. Rogers, J. Am. Chem. Soc. 2002, 124, 4974–4975

[5] R. S. Payal, K. K. Bejagam, A. Mondal, S. Balasubramanian, J. Phys. Chem. B 2015, 119, 1654–1659

[6] D. H. Zaitsau, A. V. Yermalayeu, V. N. Emel'yanenko, S. Butler, T. Schubert, S. P. Verevkin, J. Phys. Chem. B 2016, 120, 7949–7957

[7] D. H. Zaitsau, M. Kaliner, S. Lerch, T. Strassner, V. N. Emel'yanenko, S. P. Verevkin, Z. Anorg. Allg. Chem. 2017, 643, 114–119

[8] A. V. Yermalayeu, D. H. Zaitsau, M. Loor, J. Schaumann, V. N. Emel'yanenko, S. Schulz, S. P. Verevkin, Z. Anorg. Allg. Chem. 2017, 643, 81–86

[9] M. A. Varfolomeev, A. A. Khachatrian, B. S. Akhmadeev, B. N. Solomonov, A. V. Yermalayeu, S. P. Verevkin, J. Solution Chem. 2015, 44, 811–823

[10] D. H. Zaitsau, A. V. Yermalayeu, S. P. Verevkin, J. E. Bara, D. A. Wallace, Thermochim. Acta 2015, 622, 38–43

[11] D. H. Zaitsau, M. A. Varfolomeev, S. P. Verevkin, A. D. Stanton, M. S. Hindman, J. E. Bara, J. Chem. Thermodyn. 2016, 93, 151–156. DOI: 10.1016/j.jct.2015.09.033

[12] S. P. Verevkin, D. H. Zaitsau, V. N. Emel'yanenko, R. V. Ralys, A. V. Yermalayeu, C. Schick, Thermochim. Acta 2013, 562, 84–95

[13] D. H. Zaitsau, A. V. Yermalayeu, S. P. Verevkin, J. E. Bara, A. D. Stanton, Ind. Eng. Chem. Res. 2013, 52, 16615–16621. DOI: 10.1021/ie402664c

[14] S. P. Verevkin, D. H. Zaitsau, V. N. Emel'yanenko, A. V. Yermalayeu, C. Schick, H. Liu, E. J. Maginn, S. Bulut, I. Krossing, R. Kalb, J. Phys. Chem. B 2013, 117, 6473–6486

[15] M. Krannich, F. Heym, A. Jess, Chem. Eng. Technol. 2016, 39, 343–353

[16] F. Heym, W. Korth, J. Thiessen, C. Kern, A. Jess, Chem. Ing. Tech. 2015, 87, 791–802

[17] D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, R. L. Nuttall, J. Phys. Chem. Ref. Data 1982, 11, Suppl. 2-392

[18] S. P. Verevkin, D. H. Zaitsau, V. N. Emel'yanenko, A. Heintz, J. Phys. Chem. B 2011, 115, 12889–12895

[19] G. Sauerbrey, Z. Phys. 1959, 155, 206–222

[20] Y. U. Paulechka, D. H. Zaitsau, G. J. Kabo, A. A. Strechan, Thermochim. Acta 2005, 439. DOI: 10.1016/j.tca.2005.08.035

[21] D. H. Zaitsau, G. J. Kabo, A. A. Strechan, Y. U. Paulechka, A. Tschersich, S. P. Verevkin, A. Heintz, J. Phys. Chem. A 2006, 110, 7303–7306

[22] M. A. A. Rocha, C. F. R. A. C. Lima, L. R. Gomes, B. Schröder, J. A. P. Coutinho, I. M. Marrucho, J. M. S. S. Esperança, L. P. N. Rebelo, K. Shimizu, J. N. Canongia Lopes, L. M. N. B. F. Santos, J. Phys. Chem. B 2011, 115, 10919–10926

[23] M. A. A. Rocha, L. M. N. B. F. Santos, Chem. Phys. Lett. 2013, 585, 59–62

[24] M. A. A. Rocha, F. M. S. Ribeiro, B. Schröder, J. A. P. Coutinho, L. M. N. B. F. Santos, J. Chem. Thermodyn. 2014, 68, 317–321

[25] M. A. A. Rocha, J. A. P. Coutinho, L. M. N. B. F. Santos, J. Chem. Phys. B 2012, 116, 10922–10927

[26] A. V. Yermalayeu, D. H. Zaitsau, V. N. Emel'yanenko, S. P. Verevkin, J. Solution Chem. 2015, 44, 754–768

[27] M. J. Frisch et al., Gaussian 09, Revision A.02, Gaussian Inc, Wallingford, CT 2009

[28] S. P. Verevkin, V. N. Emel'yanenko, R. Notario, M. V. Roux, J. S. Chickos, J. F. Liebman, J. Phys. Chem. Lett. 2012, 3, 3454–3459

[29] L. A. Curtiss, P. C. Redfern, K. Raghavachari, V. Rassolov, J. A. Pople, J. Chem. Phys. 1999, 110, 4703–4709

[30] A. Riisager, R. Fehrmann, M. Haumann, P. Wasserscheid, Eur. J. Inorg. Chem. 2006, 695–706

[31] Supported Ionic Liquids: Fundamentals and Applications (Eds: R. Fehrmann, A. Riisager, M. Haumann), Wiley-VCH, Weinheim 2014

[32] D. H. Zaitsau, A. V. Yermalayeu, T. J. S. S. Schubert, S. P. Verevkin, J. Mol. Liq. 2017, 242, 951–957. DOI: 10.1016/j.molliq.2017.07.094

[33] D. H. Zaitsau, A. V. Yermalayeu, V. N. Emel'yanenko, S. P. Verevkin, U. Welz-Biermann, T. Schubert, Sci. China: Chem. 2012, 55, 1525–1531

[34] J. P. Armstrong, C. Hurst, R. G. Jones, P. Licence, K. R. J. Lovelock, C. J. Satterley, I. J. Villar-Garcia, Phys. Chem. Chem. Phys. 2007, 9, 982–990

[35] S. V. Sambasivarao, O. Acevedo, J. Chem. Theory Comput. 2009, 5, 1038–1050

[36] X. Zhong, Z. Liu, D. Cao, J. Phys. Chem. B 2011, 115, 10027–10040

[37] O. Borodin, J. Phys. Chem. B 2009, 113, 11463–11478

[38] A. Mondal, S. Balasubramanian, J. Phys. Chem. B 2014, 118, 3409–3422

[39] K. Shimizu, M. Tariq, M. F. Costa Gomes, L. P. N. Rebelo, J. N. Canongia Lopes, J. Phys. Chem. B 2010, 114, 5831–5834

[40] B. Schröder, J. A. P. Coutinho, Fluid Phase Equilib. 2014, 370, 24–33

[41] K. Swiderski, A. McLean, G. M. Gordon, D. H. Vaughan, Chem. Commun. 2004, 2178–2179

[42] A. Deyko, S. G. Hessey, P. Licence, E. A. Chernikova, V. G. Krasovskiy, L. M. Kustov, R. G. Jones, Phys. Chem. Chem. Phys. 2012, 14, 3181–3193

[43] D. H. Zaitsau, V. N. Emel'yanenko, S. P. Verevkin, A. Heintz, J. Chem. Eng. Data 2010, 55, 5896–5899

[44] V. N. Emel'yanenko, S. P. Verevkin, A. Heintz, J. Am. Chem. Soc. 2007, 129, 3930–3937

[45] V. N. Emel'yanenko, D. H. Zaitsau, S. P. Verevkin, A. Heintz, K. Voss, A. Schulz, J. Phys. Chem. B 2011, 115, 11712–11717

[46] S. P. Verevkin, V. N. Emel'yanenko, A. A. Pimerzin, E. E. Vishnevskaya, J. Phys. Chem. A 2011, 115, 1992–2004

[47] V. N. Emel'yanenko, M. A. Varfolomeev, S. P. Verevkin, K. Stark, K. Müller, M. Müller, A. Bösmann, P. Wasserscheid, W. Arlt, J. Phys. Chem. C 2015, 119, 26381–26389